A HIGH-PERFORMANCE EMBEDDED HYBRID METHODOLOGY FOR UNCERTAINTY QUANTIFICATION WITH APPLICATIONS

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Abstract. This paper presents a hybrid intrusive/nonintrusive methodology for embedding uncertainty quantification (UQ) capabilities into multiphysics simulators. The hybrid methodology advocates an approach that uses the best available UQ method for each individual physics module and employs suitable techniques to accurately represent and propagate the uncertainties through the full multiphysics simulation. Such a hybrid approach leads to tractable UQ analysis of complex applications, and potentially offers better flexibility than purely intrusive methods and higher efficiency than nonintrusive methods. Key components in such a hybrid approach include methods for forward uncertainty propagation, sensitivity analysis, dimension reduction, and data fusion. In addition, a software infrastructure is needed to provide accurate couplings of uncertainty propagation between individual modules and to manage allocation of computational loads in a parallel computing environment. As such, many mathematical and computer science challenges will have to be addressed in the development of this hybrid methodology. In this paper, we present some of these challenges and research/development directions to address them.

1. Introduction. Uncertainty quantification (UQ) is an emerging discipline that develops and applies systematic methodologies to assess the believability and predictability of simulation models in the presence of different sources of uncertainties in the models. Advances in mathematical/statistical techniques and the availability of petascale (and future exascale) computers in recent years have provided unprecedented opportunities to rigorously quantify uncertainties involving several complex procedures such as forward and inverse propagation of uncertainties, sensitivity analysis, model reduction, model validation/calibration, and risk analysis of large-scale multiphysics models. Moreover, existing computational tools can be leveraged in the UQ analysis of complex systems. Indeed, flexible computational infrastructures consisting of several independent but integrated solvers have gained popularity in modeling deterministic applications [11]. Each component of such an infrastructure performs a specific task addressing a single physical module of the problem of interest (physics hybridization) or operating on a subdivision of the computational domain (domain hybridization). This integration framework ensures that new features or updated models can be included without disrupting the entire environment and with a reasonable level of effort.

Unfortunately, leveraging existing software does not itself lead to high-performance UQ analysis of complex systems. In fact, the need to establish credibility of a numerical prediction introduces new challenges in the development of large-scale computational algorithms and tools, especially for multiphysics applications. For example, from a stochastic viewpoint of the target problem in which the uncertain inputs become random variables, algorithms and tools must be developed to propagate the uncertainties and quantify the impact of this propagation on the quantities of interest in the computation. Moreover, the most appropriate UQ method for the different physics modules must be investigated.

With respect to accuracy and ease of implementation, investigation into the most appropriate UQ methods will revolve around the two general classes of UQ analysis approaches: intrusive approaches, which require modification of existing computational tools or even development of new computational tools, and nonintrusive approaches, which do not require modification of existing tools and use existing computational tools as "blackbox" solvers. The most basic approach is nonintrusive Monte-Carlo (MC) methods. However, MC methods are often computationally inefficient because large numbers of realizations are often required to give accurate analyses. Fortunately, recent developments in both intrusive and nonintrusive stochastic expansion methods (polynomial chaos ([4], [14]), stochastic collocation ([13], [9]), low-rank approximations [2] and response surface reconstruction (Kriging [3], radial basis functions [8], and Pade-Legendre approaches [1]) have demonstrated impressive efficiency gains for some problems. These methods demonstrate how mathematical structure of the problems and the smoothness of the system responses can be exploited to give superlinear convergence [9].

In this paper, we present hybrid (or partially embedded) techniques for UQ. A hybrid UQ approach attempts to bridge the gap between the practicality of nonintrusive methods and the potential efficiency and robustness of intrusive methods. This is a natural alternative to applying a purely nonintrusive sampling approach to the full application problem. The idea is to integrate different intrusive and nonintrusive methods for the different physics modules in the multiphysics simulation, or even apply different UQ approaches to different parameters within a single-physics module. This hybrid approach is ideally compatible with current practices in multiphysics code development, namely, the use of "plug-and-play" capabilities to facilitate a natural division of physics expertise and to ensure that future model updates can be performed with minimal effort. However, one of the major issues in a hybrid approach is to accurately and stably propagate the

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uncertainties obtained from one UQ method for processing in another UQ method. The complexity of this issue is further intensified in strongly coupled multiphysics applications, since the physics coupling can lead to inaccuracies and instability. These are some of the issues that we will touch on in this paper.

The paper progresses as follows. In Section 2, we describe a simple abstract scenario exposing some of the challenges of UQ analysis for multiphysics applications and show that a mathematical framework that exploits intrinsic structures must be used to guide the hybrid UQ process. In Section 3, we describe some of the UQ components involved in the hybrid approach. These components/tasks must be performed on the individual module level and possibly on the full multiphysics system level, or at least performed on the individual module level with consideration of the effects on the full system level. In Section 4, we briefly describe some of the parallel computing advantages of the hybrid method and some of the parallel computing challenges. In Section 5, we present some preliminary numerical results for a hybrid approach applied to a one-dimensional reaction-diffusion. The uncertain parameters are the diffusion coefficient and reaction rate. This reaction-diffusion equation is solved by using an operator-splitting procedure that separately handles the diffusion and reaction physics, which allows different UQ methods to be applied to the diffusion and reaction physics. We show how this operator-splitting method relates to a mathematical framework and, from this, propose an alternative operator-splitting technique that may propagate the uncertainties better but may require more carefully designed hybrid approaches.

2. UQ Challenges in Multiphysics Simulations. Applying a UQ analysis to a multiphysics application can be challenging. The complex and often strong couplings between the different physics imply that the UQ analysis technically should be applied to the full system and not only to the separate modules. However, a full-system UQ analysis can easily become computationally intractable, especially when the total number of uncertain parameters in the full system is large. One way to achieve some tractability and to perform more robust hybrid UQ analysis is to exploit mathematical properties of the system. Using these properties to guide the UQ processing is what we call a mathematical framework for UQ analysis.

To demonstrate the value of a mathematical framework, we consider the multiphysics scenario in Figure 2.1.

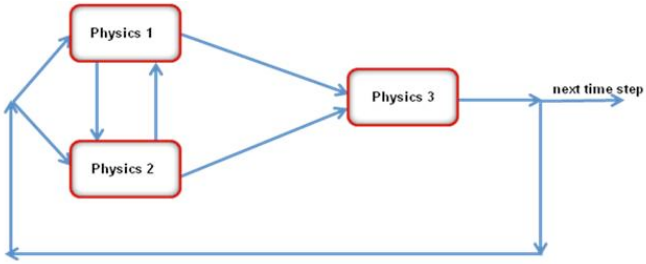

FIG. 2.1. *Simplified schematic of a multiphysics problem. Arrows between the different modules indicate coupling, and the outer cycle denotes the coupled-physics iteration required at each timestep.*

The directional arrows denote a process ordering of the coupled physics, which may have been chosen from physics intuition. We consider UQ analysis in the iterative coupled-physics cycle over one time step. Questions naturally arise: How should the uncertainties of the individual modules be represented or converted for propagation into another module? How do approximation errors affect the full simulation UQ analysis? Is there a way to quantify and minimize these effects? To answer these and other questions, a mathematical framework that requires analysis of the modeling equations can prove useful. Simply stated, the basis behind such a framework is that the propagation of information between the different modules is often described by the modeling equations themselves. Hence, a quantitative description of this propagation can be extracted from an analysis of the coupled mathematical equations. Our techniques for analyzing these systems will follow in the spirit of [15], [5] and our preliminary research [6], [7] for developing numerical solvers for systems of partial differential equations. With these techniques in hand, the strategy for the embedded hybrid UQ that we advocate is first to analyze the mathematical equations describing the multiphysics and then to exploit the extracted mathematical structures from this analysis. The goal is to use underlying structures that lead to more appropriate ways to applying the overall hybrid UQ approach than an ad hoc application of a hybrid method.

To illustrate how even a "crude" mathematical analysis can help, we consider a general multiphysics system. Intuitively, a multiphysics phenomenon describes feedback interactions propagating information between the different physics modules. Given that the feedback system describes the phenomenon accurately, its properties should be exploited to better understand the phenomenon or possibly even to simplify the description of the phenomenon. For example, suppose the feedback has a natural (i.e. physical) preferential

ordering whereby information is propagated stably. Then the phenomenon should be numerically processed following this preferential ordering. Moreover, this ordering may expose a new feedback system that is more loosely coupled and that has reduced dependency.

The feedback interactions are described by the mathematical equations modeling the phenomenon. Thus, an analysis of these equations can reveal how information is propagated. One type of analysis is to compare the "strengths" of the mathematical operators describing the individual physics modules and the intermodule interactions. This comparison can help describe how approximation errors affect the full system UQ analysis. In particular, it can help determine whether dimensional reduction in a local physics module indeed produces only negligible effects on the other physics modules. Moreover, this strength comparison can lead to (mathematical and thereby physical) preferential orderings, which correspond to reorderings of the mathematical equations and unknowns in the multiphysics system and which may reveal weak couplings between some of the physical quantities. These weak couplings can lead to hybrid UQ algorithms with higher algorithmic parallelism, because of reduced dependency.

For example, consider the multiphysics scenario depicted in Figure 2.1. For illustrative simplicity, we assume that the individual modules are linear, that the interaction between each component affects only the forcing terms of the other physics modules, that uncertainties arise only in the intraphysics modules, and that the uncertainties of the controllable/observable forcing terms have the same type of aleatory uncertainties as in their corresponding intraphysics modules. Formally, then, Figure 2.1 can be described in matrix form as

$$\begin{bmatrix} L_{11}(\omega_1) & L_{12} & L_{13} \\ L_{21} & L_{22}(\omega_2) & L_{23} \\ L_{31} & L_{32} & L_{33}(\omega_3) \end{bmatrix} \begin{pmatrix} u_1(\omega_1,\omega_2,\omega_3) \\ u_2(\omega_1,\omega_2,\omega_3) \\ u_3(\omega_1,\omega_2,\omega_3) \end{pmatrix} = \begin{pmatrix} f_1(\omega_1) \\ f_2(\omega_2) \\ f_3(\omega_3) \end{pmatrix}, \tag{2.1}$$

where ω_i denotes the random variables and L_{ij} denotes the feedback operator from module j to module i. Note that although the intramodule operators (L_{ii}) and their forcing terms (f_i) are dependent only on ω_i, the solution components inherit the different types of uncertainties through the cross-couplings. Now assume that in the appropriate norms, the extracted mathematical structures are as follows:

1. L_{12} is negligible when compared to L_{11} and L_{13}, L_{21} and L_{23} are negligible when compared to L_{22}, and L_{32} is negligible when compared to L_{31} and L_{33};
2. $\|L_{12}\| > \|L_{21}\|$ and $\|L_{32}\| > \|L_{23}\|$; and
3. $O(1) \approx \left\|(L_{11})^{-1}L_{13}\right\| << \left\|(L_{33})^{-1}L_{31}\right\|$.

Then, using structure (1), we have

$$\begin{bmatrix} L_{11}(\omega_1) & L_{12} & L_{13} \\ L_{21} & L_{22}(\omega_2) & L_{23} \\ L_{31} & L_{32} & L_{33}(\omega_3) \end{bmatrix} \approx \begin{bmatrix} L_{11}(\omega_1) & 0 & L_{13} \\ 0 & L_{22}(\omega_2) & 0 \\ L_{31} & 0 & L_{33}(\omega_3) \end{bmatrix}. \tag{2.2}$$

Furthermore, from these structures and (2.2), we can deduce the following considerations for a hybrid UQ analysis of this multiphysics system.

Parallel UQ Analysis - Structure (2) reveals that the feedback from module 2 to modules 1 and 3 (i.e., L_{12} and L_{32}, respectively) is stronger than the feedback into module 2 from modules 1 and 3 (i.e., L_{21} and L_{23}, respectively). Thus, system (2.1) should be reordered as

$$\begin{bmatrix} L_{22}(\omega_2) & L_{21} & L_{23} \\ L_{12} & L_{11}(\omega_1) & L_{13} \\ L_{32} & L_{31} & L_{33}(\omega_3) \end{bmatrix} \approx \begin{bmatrix} L_{22}(\omega_2) & 0 & 0 \\ 0 & L_{11}(\omega_1) & L_{13} \\ 0 & L_{31} & L_{33}(\omega_3) \end{bmatrix}, \tag{2.3}$$

where the right system is obtained by using (2.2). From this re-ordering, we see that after an initial UQ bootstrapping of the multiphysics system, the UQ analysis of module 2 can be decoupled from the UQ analysis of the other modules. Thus, additional local UQ analysis of module 2 can be performed in parallel with additional UQ analyses of the other modules, which should be performed in a coupled manner. Of course, since all modules are coupled in the actual multiphysics system, the results of the UQ analysis of module 2 must eventually be synchronized back into the full system and vice versa, but at less frequency than UQ propagation is required between modules 1 and 3.

Sensitivity Analysis and Dimension Reduction - Suppose some type of sensitivity analysis is performed on module 1 by perturbing a subset of the uncertain parameters in operator L_{11}. Let $\tilde{u}_1$ denote the perturbed solution. If this solution component differs only slightly from the unperturbed solution, then one may conclude that these perturbed parameters are irrelevant; that is, dimension reduction can be performed by

eliminating these parameters. Although this conclusion is valid for the intrinsic uncertainties in module 1, it may not be valid in the full model since the effects of this dimension reduction (the change in the induced uncertainties) can substantially impact the solution components for the other modules during the iterative cycling over the full system. Indeed, using structure (3.) and denoting the perturbed solution by $\tilde{u}_3$, we have

$$\|u_3 - \tilde{u}_3\| \leq \left\|(L_{33})^{-1} L_{31}\right\| \|u_1 - \tilde{u}_1\|, \tag{2.4}$$

which can be large. That is, although the difference between dimension-reduced $\tilde{u}_1$ and u_1 is small, its effect on module 3 can be large. On the other hand, a dimension reduction for module 3 may not impact module 1 as dramatically.

The above example shows how a mathematical framework can help guide UQ analysis of multiphysics systems. However, the assumptions of this example are dramatic simplifications of realistic multiphysics systems. Multiphysics problems are generally nonlinear, with more complex interactions and uncertainty dependence. Nevertheless, using a mathematical framework to help guide the UQ analysis is a first step in making this analysis tractable.

3. Components for Hybrid UQ Analysis. With the aid of a mathematical framework, UQ analysis for complex systems will be more achievable. With or without this guidance, though, many UQ components must be performed within a hybrid approach. We summarize some of them, some of which have already been referred to in the previous sections.

Representations of Uncertainties - Irrespective of how uncertainties are represented within each physics module, the uncertainties must be propagated to the other modules in a base format recognizable by other physics modules. Some of the possible formats/representations are statistical moments, probability distributions, local sensitivity information, polynomial chaos expansions, and other functional forms. In evaluating the suitability of the representation, factors that must be considered include the following: Does the representation provide enough uncertainty information for different UQ processing? Does the representation permit different probability distributions for the uncertain parameters? Does the representation allow easy and accurate conversion to the intra-module representations? For example, local sensitivity information may not be suitable because strong nonlinearities in the multiphysics system can render this local information irrelevant.

Forward Uncertainty Propagation - Given a set of uncertain parameters and their probability distributions, forward uncertainty propagation derives the corresponding model output distribution. This requires accurate uncertainty representations and efficient algorithms to propagate the uncertainties, for example, efficient methods to solve systems of equations, which are dependent on the uncertainties. For high dimensional models, dimension reduction techniques can help reduce the computational cost.

Dimension Reduction and Sensitivity Analysis - The task of quantifying uncertainties suffers from the curse-of-dimensionality problem; in other words, the computational complexity grows exponentially with the number of independent sources of uncertainties. For example, without any prior knowledge of the model's output behavior in the uncertain parameter space, the computational cost for fully exploring this parameter space is $\mathrm{O}(k^m)$, where m and k are the number of uncertain parameters and the number of points required to resolve each parameter dimension, respectively. Reducing m without destroying the quantitative validity of the model is generally called dimension reduction. Dimension reduction is especially important for multiphysics applications because the total number of uncertain parameters is often large.

One dimension reduction technique is to use *local* sensitivity analysis. For general nonlinear problems such as those in multiphysics simulations, *global* screening techniques are preferred [10] to remove insignificant parameters from the final UQ study.

Data Fusion - Computational models representing complex physical systems naturally have approximation errors. An approach often used to "improve" the models is to assimilate measured data. This may involve a measurement model that relates the actual states of the physical systems and the measured observables. The defect between the actual measurements and the computed measurements generated by evaluating the measurement model at the computed states can be used to calibrate the computational model. This process is called data fusion/assimilation. Traditionally, data fusion has been used to calibrate engineering models using data collected in dedicated experiments intended to reproduce a subset of the operating conditions in the system. This process is highly dependent on the availability of sufficient data to characterize the invariably large number of parameters in the computational models. Moreover, the presence of uncertainty in the measurements and the mismatch between model parameters and measured quantities requires either

a regularization procedure or a comprehensive stochastic inference process [12].

These and other UQ components must be conducted both in the physics module level and the full multiphysics system level. A major challenge is determine stable and accurate methods to perform these at both levels. Another challenge is to perform these efficiently, particularly performing them on parallel computers.

4. Parallel Computing Issues. In order to ensure fast simulation of a hybrid UQ method, high-performance computers, such as modern extreme-scale machines, are needed. The hybrid embedded UQ approach has features that are attractive for extreme-scale computing. Because of a blending of intrusive and nonintrusive methods, the hybrid approach inherits the good parallel features of some methods and reduces the poor parallel features of other methods. For example, by incorporating nonintrusive, sampling-based methods some embarrassingly parallel features are inherited by the hybrid approach. On the other hand, using an intrusive method such as polynomial chaos on some of the modules not only can reduce the total number of multiphysics simulations but also avoid having to solve extremely large matrix systems if a polynomial chaos method were used on the full system model. Smaller size matrix systems must still be solved, but they can be solved using appropriately designed preconditioners. Indeed, being able to use these preconditioners will reduce the number of global processor synchronizations that would be needed for solving larger matrix systems. Thus, interspersing nonintrusive and intrusive methods in an optimal way within a hybrid approach promises higher efficiency and more effective use of next-generation computers.

This is a general statement. But it is not hard to imagine some of the particular parallel computing issues. We mention one that arises not only for UQ analysis of multiphysics problems but also in multiphysics simulation itself. It is the processor partitioning. High efficiency will greatly depend on how the problem is partitioned into the processor nodes of an extreme-scale computer. A good partition must minimize long-distance processor communication. Whereas this may be somewhat accomplished in the parallelization of a physics module, this may not be completely achievable in the parallelization of the full multiphysics system. With respect to the hybrid approach, the processor partitioning must be carefully designed to avoid long-distance communication when propagating the uncertainties between the modules. This requirement means that the partitions generally must be determined not by what is best for one module but, rather, on what is best for all the modules together. Appropriate processor mapping schemes that ensure minimal long-distance communication for the full system must be considered.

5. Numerical Study. The main objective of this numerical study is to present a capability for propagating uncertainties in a hybrid environment using a simple time-dependent reaction diffusion equation as an example. With the aid of a generic software infrastructure, we analyze an algorithm that can propagate global uncertainties while keeping the uncertainty treatment of the reaction and diffusion modules separate. We also relate this numerical example to a mathematical framework.

The test problem is the following one-dimensional reaction-diffusion equation

$$\left\{\begin{array}{lll} \frac{\partial u}{\partial t} & = D\frac{\partial^2 u}{\partial x^2} - Ku & 0 < x < 1, \quad 0 < t \le T \\ u(0,t) & = u(1,t) = 0 & t \ge 0 \\ u(x,0) & = f(x) & 0 \le x \le 1, \end{array}\right. \tag{5.1}$$

where D and K are second-order random variables describing spatially independent diffusion and reaction rates, respectively. Problem (5.1) is a simplification of the reaction-convection-diffusion equation modeling subsurface transport and reaction flow for multispecies concentrations. Here, we consider only one specie and no convection.

The solution to the deterministic form of (5.1) is

$$u(x,t) = \sum_{n=1}^{\infty} f_n \sin(n\pi x) e^{-\left[(n\pi)^2 D + K\right]t}, \quad f_n = 2\int_0^1 f(x)\sin(n\pi x)dx.$$

Here, we take $f(x) = \sin(m\pi x)$ so that the solution is

$$u(x,t) = \sin(m\pi x) e^{-\left[(m\pi)^2 D + K\right]t}.$$

We note that this simplification will reduce the complexity of the uncertainty propagation.

To numerically solve the stochastic form of (5.1), an operator splitting technique is used. To be precise, an implicit stochastic expansion is first assumed, and then the stochastic system is solved by operator splitting. This splitting separates the diffusion and reaction processes, which is a natural decomposition for these characteristically different processes. Moreover, this splitting will permit more appropriate solution

methods to be used for the diffusion and reaction. Now, at timestep $(n+1)$ for subinterval $\left[t^n, t^{n+1}\right]$, the operator splitting method involves solving the diffusion and reaction equations

$$\begin{cases} \frac{\partial u^d}{\partial t} & = D\frac{\partial^2 u^d}{\partial x^2} & 0<x<1, \quad t^n < t \le t^{n+\frac{1}{2}} \\ u^d(0,t) & = u^d(1,t) = 0 & t^n \le t \le t^{n+\frac{1}{2}} \\ u^d(x,t^n) & = u^r(x,t^n) & 0 \le x \le 1, \end{cases} \tag{5.2}$$

and

$$\begin{cases} \frac{\partial u^r}{\partial t} & = Ku^r & 0<x<1, \quad t^{n+\frac{1}{2}} < t \le t^{n+1} \\ u^r(0,t) & = u^r(1,t) = 0 & t^{n+\frac{1}{2}} \le t \le t^{n+1} \\ u^r(x,t^{n+\frac{1}{2}}) & = u^d(x,t^{n+\frac{1}{2}}) & 0 \le x \le 1 \end{cases} \tag{5.3}$$

with coupling occurring only through the initial conditions of each system. In our experiments, an intrusive polynomial chaos (PC) method is used on diffusion equation (5.2), and a nonintrusive sampling method is used on reaction equation (5.3). The developed computational framework allows the diffusion and reaction solvers to be implemented independently and without knowledge of each other. The initial-condition coupling is realized by passing the PC coefficients of the diffusion module to the reaction module and by passing PC coefficients obtained by a Legendre regression of the reaction solution to the diffusion module. Table 5.1 tabulates some results for $m = 5, T = 2$, $D \in [0.0001, 0.001]$ and $K \in [0.1, 0.5]$ both having uniform distributions, (5.2) spatially discretized by center-differencing and temporal discretized by backward Euler, and (5.3) solved analytically over each time subinterval. Also, the time and spatial meshsizes are $\Delta t = 0.01$ and $\Delta x = \frac{1}{256}$, respectively, and the output of interest is the solution at $(x,t) = (0.5, 2)$. Table 5.1 compares the results of a purely PC method for solving (5.1) to results of the hybrid operator splitting method.

TABLE 5.1
Comparison of Errors and Times for Test Case 1

	PC only		Hybrid	
PC Order	$u(0.5,2)$/rms error	time (s)	$u(0.5,2)$/rms error	time (s)
1	1.61e-3/4.91e-4	8.0	2.57e-2/7.83e-3*	10.5
2	1.86e-3/5.66e-4	10.5	1.58e-4/4.83e-5	14.5
3	1.86e-3/5.66e-4	13.5	1.32e-3/4.01e-4	23.5
4	1.86e-3/5.66e-4	16.5	2.90e-4/8.86e-5	29.0
5	1.86e-3/5.66e-4	20.5	2.83e-4/8.62e-5	40.0
6	1.86e-3/5.66e-4	25.5	2.87e-4/8.76e-5	46.0
$D = [0.0001, 0.001], K = 0.1, 0.5]$ $u(0.5,2)$ - error for the mean of $u(x = 0.5, t = 2)$ (*) sample size used = 5 instead of 3 rms error - root-mean-square error for the means at $x = [0,1]$				

The following observations can be deduced:

- The hybrid method attains smaller errors than the purely intrusive PC method when p is sufficiently large, which may be due to solving the reaction equation analytically.
- The execution time for the hybrid method is longer than that for the purely intrusive PC method. But further investigation of the hybrid method shows that this is due to the construction of the PC coefficients using Legendre regression in the reaction module. In order to reduce the timings for the hybrid method, some code optimization can be performed, or a simple projection of the reaction solution onto the PC basis functions of the diffusion module can be used.
- In order to obtain the accuracy of the hybrid method, the purely intrusive PC method requires smaller timesteps. With finer timesteps, the hybrid method can timewise outperform the purely intrusive method; for example, for $\Delta t = 0.002$, the purely intrusive method gives $u(x = 0.5, t = 2)$ and rms errors of $4.4E-4$ and $1.3E-4$ for $p = 6$ but requiring 125 seconds.

The above operator=splitting method can be related to a mathematical framework for the UQ analysis of (5.1). Processing the diffusion system first, the operator split equations (5.2) and (5.3) convert (5.1) to a system with operator

$$\begin{bmatrix} \frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2} & 0 \\ I.C. & \frac{\partial}{\partial t} + K \end{bmatrix} \begin{pmatrix} u^d_{n+\frac{1}{2}} \\ u^r_{n+1} \end{pmatrix} \tag{5.4}$$

defined over the time interval $\left(t^n, t^{n+1}\right]$. Here $I.C.$ denotes the initial condition coupling the reaction module to the diffusion module. From (5.4), we see that the operator splitting leads to a weakly coupled system that general will not dramatically amplify the errors in the diffusion process. In fact, when the operator split iteration is bootstrapped with the initial condition $u(x,0) = \sin(m\pi x)$, the analytic solution of (5.4) is

$$u^d_{n+\frac{1}{2}} = \sin(m\pi x) e^{-\left[(m\pi)^2 D t^{n+\frac{1}{2}} + K t^n\right]} \tag{5.5}$$

$$u^r_{n+1} = \sin(m\pi x) e^{-\left[(m\pi)^2 D t^{n+\frac{1}{2}} + K t^{n+1}\right]}, \tag{5.6}$$

from which we can get an idea on the uncertainty and error propagation. Of course, this propagation is more complex if the initial condition is more general and if the uncertainty parameters are random fields.

A concern that may arise with regard to this operator split method is whether the uncertainty information of one module is sufficiently propagated to other module via through the initial conditions only. This concern will be more relevant when the problem involves uncertainty fields. To represent the uncertainty propagation more strongly, one can reduce the time step that will result in longer simulation time. Alternatively, one can include a time-lagged reaction term to the diffusion equation and a time-lagged diffusion term to the reaction equation. In the time interval $\left(t^n, t^{n+1}\right]$, the system operator is

$$\begin{bmatrix} \frac{\partial}{\partial t} - D\frac{\partial^2}{\partial x^2} & 0 \\ I.C. + \left(-D\frac{\partial^2}{\partial x^2}\right) & \frac{\partial}{\partial t} + K \end{bmatrix} \begin{pmatrix} u^d_{n+\frac{1}{2}} \\ u^r_{n+1} \end{pmatrix}, \tag{5.7}$$

which leads to more complex uncertainty and error propagation. Moreover, the diffusion and reaction modules now require solving nonhomogeneous equations. The analytic solution for the reaction module will have the form

$$u^r_{n+1} = \left[u^d_{n+\frac{1}{2}} + \int -D\frac{\partial^2 u^d_{n+\frac{1}{2}}}{\partial x^2} e^{Kt} dt \right] e^{-Kt}, \tag{5.8}$$

and the analytic solution of the diffusion module will involve a finite sine transform. From (5.8), we expect a complex propagation of the uncertainty and errors. Thus, the hybrid method for system (5.7) must be more carefully designed and analyzed.

6. Final Remarks. The vision of our research is to develop a technology for building practical UQ-ready multiphysics simulation codes founded on sound mathematics and leading to high parallel efficiency. The technology is based on a hybrid UQ approach, which employs both intrusive and nonintrusive methods in a flexible manner within a simulation model. We have identified some challenges for building this capability, and our proposed research directly addresses these challenges. If successful, this technology will be of great value to scientists for building UQ-ready codes, understanding the flow of uncertainties, and thus improving their simulation models. This work also helps to advance UQ mathematics, and the hybrid framework will be a candidate for "co-design" in designing the next-generation exascale computers.

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